

=> FILE REG

FILE 'REGISTRY' ENTERED ON 31 AUG 2007

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=> D HIS

L1 FILE 'LREGISTRY'
STR

L2 FILE 'REGISTRY'
50 S L1

L3 FILE 'LREGISTRY'
STR L1
E NITROXIDE/CN
L4 1 S E3
E NITROXIDE
L5 57 S E3
L6 STR L3

L7 FILE 'REGISTRY'
28 S L6

L8 FILE 'LREGISTRY'
STR L6

L9 FILE 'REGISTRY'
7 S L8

L10 FILE 'LREGISTRY'
E THIOISOCYANATE
4 S E3
L11 STR L8

L12 FILE 'REGISTRY'
7 S L11

L13 FILE 'HCAPLUS'
282 S NESVADBA ?/AU
L14 4515 S ?ALKOXYAMIN? OR ?ETHOXYAMIN? OR ?PROPOXYAMIN?
L15 20 S L13 AND L14
L16 10617 S NITROXIDE#
L17 17 S L13 AND L16
L18 8 S L15 AND L17
SEL L18 1-8 RN

FILE 'REGISTRY'

L19 250 S E1-E250
 L20 8289 S ?NITROXID?/CNS
 L21 7 S L19 AND L20
 L22 2460 S L11 FUL
 SAV L22 TRU693/A

FILE 'HCA'

L23 1196 S L22
 L24 202207 S TRANSITION?(2A) (METAL#### OR SALT#)
 L25 96610 S METAL#### (2A) SALT#
 L26 59 S L23 AND (L24 OR L25)
 L27 57 S L23 AND L24
 L28 4 S L23 AND L25
 L29 0 S L26 AND L14

FILE 'REGISTRY'

L30 37531 S C H N/ELF AND 3/ELC.SUB AND NO RSD/FA

FILE 'HCA'

L31 454650 S L30
 L32 4 S L26 AND L31
 L33 4 S L23 AND L14
 L34 92 S L23 AND L31
 L35 4 S L34 AND (L24 OR L25)

FILE 'REGISTRY'

L36 650567 S C H N/ELF AND 3/ELC.SUB
 L37 39190 S L36 AND 2<ELR.HC

FILE 'HCA'

L38 333287 S L37
 L39 3 S L26 AND L38
 L40 79 S L23 AND L38
 L41 3 S L40 AND (L24 OR L25)
 L42 8 S L32 OR L33 OR L35 OR L39 OR L41

FILE 'REGISTRY'

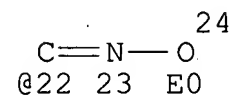
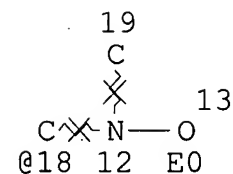
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 L11 STR

N~C~S
1 2 @3

G1 6

G2 9

G3 30



VAR G1=3/X
VAR G2=3/X/18/22
VAR G3=18/22

NODE ATTRIBUTES:

HCOUNT IS E0 AT 13
HCOUNT IS E0 AT 24
NSPEC IS RC AT 18
NSPEC IS RC AT 19
NSPEC IS RC AT 22
CONNECT IS E2 RC AT 2
CONNECT IS E1 RC AT 13
CONNECT IS E1 RC AT 24
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L22 2460 SEA FILE=REGISTRY SSS FUL L11

100.0% PROCESSED 444373 ITERATIONS (3 INCOMPLETE) 2460 ANSWERS
SEARCH TIME: 00.00.05

=> FILE HCA

FILE 'HCA' ENTERED ON 31 AUG 2007

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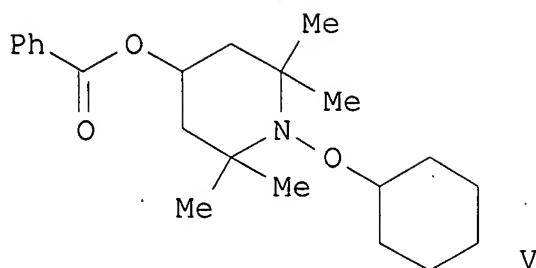
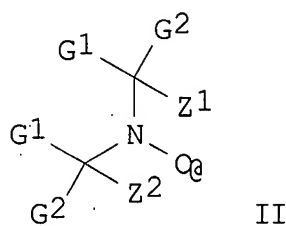
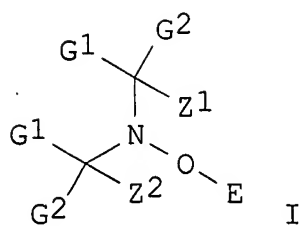
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=> D L42 1-8 CBIB ABS HITSTR HITIND

L42 ANSWER 1 OF 8 HCA COPYRIGHT 2007 ACS on STN

142:155822 Hydrogen peroxide catalyzed alkoxylation of nitroxyl compounds to sterically hindered N-hydrocarbyloxyamines, especially N-hydrocarbyloxy-2,2,6,6-piperidines. Galbo, James Peter; Detlefsen, Robert Edward (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2005005388 A1 20050120, 57 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2004-EP51352 20040705. PRIORITY: US 2003-486994P 20030714.

GI

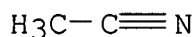


- AB The invention is directed to the prepn. of sterically hindered N-hydrocarbyloxyamines I, well-known as thermal and light stabilizers, by alkoxylation of hindered amine N-oxyl compds. II with a hydrocarbon solvent contg. no activated hydrogen atoms in the presence of hydrogen peroxide or a hydrogen peroxide equiv., a catalytic amt. of a peroxide decompg. **transition metal salt, metal oxide, or metal-ligand complex**, an inert cosolvent and an optionally acid [wherein G1, G2 = independently alkyl or are together pentamethylene; Z1, Z2 = each Me, or Z1 and Z2 together form a (un)substituted linking moiety; E = alkyl, cycloalkyl, bicycloalkyl, etc; with the provision that in the hydrocarbon, no carbon atom attached to an arom. ring is substituted by H]. The advantages include use of less toxic solvents, cheap oxidn. reagents, absence of additives, and lower reaction temp. Thus, dropwise addn. at reflux over 4.75 h of 50% aq. H2O2 to a preheated mixt. contg. FeSO4•7H2O (III), CH3SO3H (IV), 1-oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine, acetonitrile and hexane, with addnl. portions of III and IV added after 1 and 2.25 h after the peroxide addn. started, gave 65% V.
- IT **75-05-8**, Acetonitrile, uses (cosolvent; prepn. of sterically hindered N-hydrocarbyloxyamines, in particular N-hydrocarbyloxy-2,2,6,6-piperidines, by hydrogen

peroxide catalyzed alkoxylation of N-oxyl compds.)

RN 75-05-8 HCA

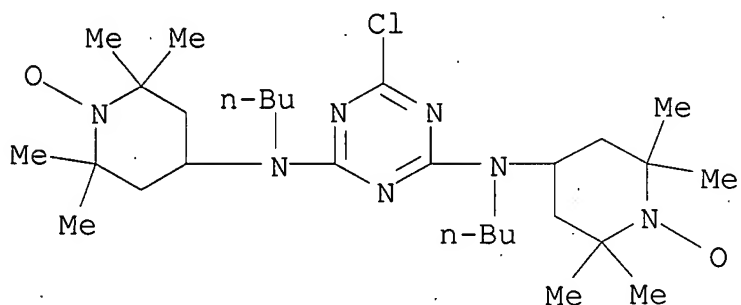
CN Acetonitrile (CA INDEX NAME)



IT **290821-91-9**, 2-Chloro-4,6-bis[N-(1-oxyl-2,2,6,6-tetramethylpiperidin-4-yl)butylamino]-s-triazine (nitroxyl compd. starting material; prepn. of sterically hindered N-hydrocarbyloxyamines, in particular N-hydrocarbyloxy-2,2,6,6-piperidines, by hydrogen peroxide catalyzed alkoxylation of N-oxyl compds.)

RN 290821-91-9 HCA

CN 1-Piperidinyloxy, 4,4'-[(6-chloro-1,3,5-triazine-2,4-diyl)bis(butylimino)]bis[2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



IC ICM C07D211-94

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 45

IT Hydroperoxides

Oxides (inorganic), uses

Salts, uses

Transition metals, uses

(prepn. of sterically hindered N-hydrocarbyloxyamines, in particular N-hydrocarbyloxy-2,2,6,6-piperidines, by hydrogen peroxide catalyzed alkoxylation of N-oxyl compds.)

IT 67-56-1, Methanol, uses **75-05-8**, Acetonitrile, uses

(cosolvent; prepn. of sterically hindered N-hydrocarbyloxyamines, in particular N-hydrocarbyloxy-2,2,6,6-piperidines, by hydrogen peroxide catalyzed alkoxylation of N-oxyl compds.)

IT 3225-26-1, 1-Oxyl-4-benzoyloxy-2,2,6,6-tetramethylpiperidine

22977-67-9, 1-Oxyl-4-Octadecanoyloxy-2,2,6,6-tetramethylpiperidine

290821-91-9, 2-Chloro-4,6-bis[N-(1-oxyl-2,2,6,6-tetramethylpiperidin-4-yl)butylamino]-s-triazine

(nitroxyl compd. starting material; prepn. of sterically hindered N-hydrocarbyloxyamines, in particular N-hydrocarbyloxy-2,2,6,6-

piperidines, by hydrogen peroxide catalyzed alkoxylation of N-oxyl compds.)

L42 ANSWER 2 OF 8 HCA COPYRIGHT 2007 ACS on STN

139:350973 The use of PROXYL nitroxides in nitroxide-mediated polymerization. Cameron, Neil R.; Bacon, Catherine A.; Reid, Alistair J. (Department of Chemistry, University of Durham, Durham, DH1 3LE, UK). ACS Symposium Series, 854 (Advances in Controlled/Living Radical Polymerization), 452-465 (English) 2003. CODEN: ACSMC8. ISSN: 0097-6156. Publisher: American Chemical Society.

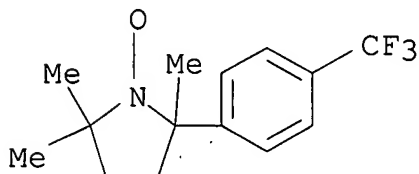
AB The use of **alkoxyamines** derived from substituted PROXYL nitroxides is studied and performance is compared to analogous species obtained from TEMPO. PROXYLs are found to have significant differences relative to TEMPO: more rapid styrene polymn.; the ability to bring about the living polymn. of Bu acrylate; and a lower propensity to undergo disproportionation. The latter is suggested to be the key parameter producing the different behavior of PROXYL nitroxides.

IT **328311-58-6**

(use of PROXYL nitroxides in nitroxide-mediated polymn.)

RN 328311-58-6 HCA

CN 1-Pyrrolidinyloxy, 2,2,5-trimethyl-5-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

IT Amines, uses

(**alkoxyamine** derivs.; use of PROXYL nitroxides in nitroxide-mediated polymn.)

IT 3229-53-6 62539-49-5 154554-67-3 185055-65-6

328311-58-6 328311-59-7 328311-60-0 328311-61-1

328311-62-2 328311-63-3 618881-90-6

(use of PROXYL nitroxides in nitroxide-mediated polymn.)

L42 ANSWER 3 OF 8 HCA COPYRIGHT 2007 ACS on STN

134:208210 Studies on controlled radical polymerization using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**. Cameron, Neil R.; Reid, Alistair J.; Span, Piet; Bon, Stefan A. F.; Van Es, J. J. G. Steven; German, Anton L. (Department of Chemistry, University of Durham, Durham, DH1 3LE, UK). Macromolecular Chemistry and Physics, 201(17), 2510-2518 (English) 2000. CODEN:

MCHPES. ISSN: 1022-1352. Publisher: Wiley-VCH Verlag GmbH.

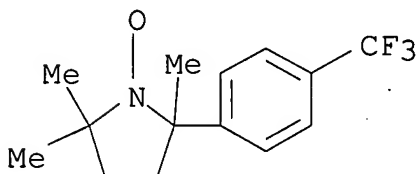
AB 2,2',5,5'-Tetramethylpyrrolidine-N-oxyl (PROXYL) and derivs. bearing one α -aryl substituent (Ph, p-CF₃Ph, p-Me₂NPh) were prepd. and converted to **alkoxyamines** by reaction with di-tert-Bu peroxalate (DTBPO) and excess styrene. Both the nitroxides (plus DTBPO as a radical source) and **alkoxyamines** were investigated in the controlled radical polymn. (CRP) of styrene, and their behavior was compared to that of TEMPO. Polymn. mediated by each nitroxide displayed a linear relationship between mol. wt. and conversion, producing material of low poly-dispersity indicating a controlled process. However, a comparison of kinetic behavior was complicated by the unknown concn. of active species present. Polymns. with preformed **alkoxyamines** at a known concn. also displayed controlled behavior (poly-dispersities 1.25-1.5), and an influence of nitroxide substituent on the overall rate of polymn. could be detd. PROXYL and the dimethylanilino-substituted nitroxide gave similar CRP rates to TEMPO, whereas a Ph or (to a lesser extent) p-CF₃Ph substituent resulted in significantly faster reactions. These results are discussed in terms of the likely steric and electronic influence of substituents on the nitroxide radical center, and the resulting influence on polymn. rate. It is concluded that the steric bulk of the Ph substituent is the most likely cause of the rate enhancement displayed by the corresponding mediator.

IT 328311-58-6P

(in **alkoxyamine** prepn.; controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

RN 328311-58-6 HCA

CN 1-Pyrrolidinyloxy, 2,2,5-trimethyl-5-[4-(trifluoromethyl)phenyl]-
(9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)

ST PROXYL nitroxide **alkoxyamine** catalyst radical polymn
styrene; safety detonation butyl peroxalate catalyst polymn styrene

IT Amines, preparation

(**alkoxyamines**; controlled radical polymn. of styrene
using 5-membered cyclic PROXYL nitroxides and corresponding
alkoxyamines)

IT Polymerization catalysts
Steric effects

Substituent effects

(controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT Nitroxides

(controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT Safety

(detonation; controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT 185055-65-6P 328311-60-0P 328311-61-1P 328311-62-2P
328311-63-3P

(controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT 9003-53-6P, Polystyrene

(controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT 3229-53-6P 62539-49-5P **328311-58-6P** 328311-59-7P

(in **alkoxyamine** prepn.; controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

IT 100-42-5, Styrene, reactions 1876-22-8, Di-tert-butyl peroxalate
2564-83-2, TEMPO 4567-18-4, 2,5,5-Trimethyl-1-pyrroline-1-oxide
(in **alkoxyamine** prepn.; controlled radical polymn. of styrene using 5-membered cyclic PROXYL nitroxides and corresponding **alkoxyamines**)

L42 ANSWER 4 OF 8 HCA COPYRIGHT 2007 ACS on STN

133:223565 Hydroxy-substituted, N-alkoxy, hindered heterocyclic amines for stabilizers for polymers and coatings. Galbo, James Peter; Capocci, Gerald Anthony; Cliff, Nancy Nase; Detlefsen, Robert Edward; Difazio, Michael Peter; Ravichandran, Ramanathan; Solera, Peter Shelsey; Grace, Henry Clanton; Kuell, Christopher (Ciba Specialty Chemicals Holding Inc., Switz.). Ger. Offen. DE 10008367 A1 20000831, 96 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2000-10008367 20000223. PRIORITY: US 1999-257711 19990225; US 1999-315704 19990520.

AB The title compds. having ≤ 3 OH on the alkoxy substituent group and are useful for stabilizing polyolefins and coatings against heat, light, and O where similar compds. having no OH groups on the alkoxy substituent and higher basicity are not as useful as stabilizers. These compds. are manufd. by reaction of the appropriate N-oxyl compd. with an alc. in presence of a peroxide or an org. hydroperoxide and a catalytic quantity of a **metal salt** or a **metal** ligand complex. Thus, heating 23.5 g 1-oxyl-2,2,6,6-tetramethylpiperidin-4-one with 14 g cyclohexanol in cyclohexane in the presence of H₂O₂, FeCl₂·4H₂O 3 h at 40°, adding more H₂O₂, heating 7 h at 40°, cooling

to room temp., adding 5 g Na₂SO₃, and heating at 60° to decomp. the excess H₂O₂ gave 16 g 1-(hydroxycyclohexyloxy)-2,2,6,6-tetramethylpiperidin-4-one.

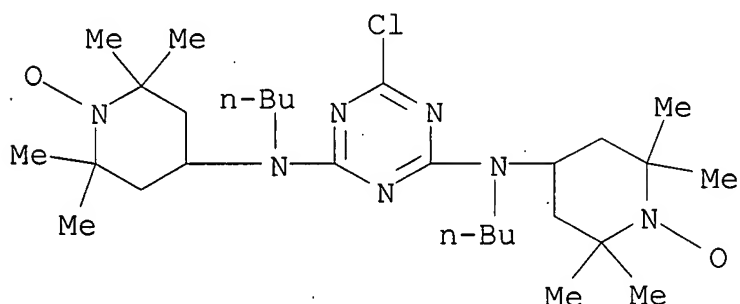
IT **111-86-4**, Octylamine **10563-26-5**,
N,N'-Bis(3-aminopropyl)ethylenediamine **290821-91-9**
(stabilizer precursor; hydroxy-substituted, N-alkoxy, hindered heterocyclic amines for stabilizers for thermoplastic polymers and coatings)
RN 111-86-4 HCA
CN 1-Octanamine (CA INDEX NAME)

H₂N-(CH₂)₇-Me

RN 10563-26-5 HCA
CN 1,3-Propanediamine, N1,N1'-1,2-ethanediylbis- (CA INDEX NAME)

H₂N-(CH₂)₃-NH-CH₂-CH₂-NH-(CH₂)₃-NH₂

RN 290821-91-9 HCA
CN 1-Piperidinyloxy, 4,4'-[(6-chloro-1,3,5-triazine-2,4-diyl)bis(butylimino)]bis[2,2,6,6-tetramethyl- (9CI) (CA INDEX NAME)



IC ICM C07D211-94
ICS C07D401-06; C07D401-14; C07D493-10; C07D493-20; C07D401-04;
C09D011-02; C09D005-32
CC 37-6 (Plastics Manufacture and Processing)
Section cross-reference(s): 27
IT 57-55-6, 1,2-Propanediol, reactions 67-63-0, Isopropanol, reactions 75-65-0, tert-Butanol, reactions 75-77-4, reactions 77-99-6, 2-Ethyl-2-(hydroxymethyl)-1,3-propanediol 106-69-4, 1,2,6-Hexanetriol 106-95-6, Allyl bromide, reactions 108-93-0, Cyclohexanol, reactions 110-63-4, 1,4-Butanediol, reactions 111-82-0, Methyl laurate **111-86-4**, Octylamine 112-39-0, Methyl palmitate 126-30-7 141-43-5, reactions 504-01-8, 1,3-Cyclohexanediol 504-63-2, 1,3-Propanediol 556-48-9,

1,4-Cyclohexanediol 584-03-2, 1,2-Butanediol 816-19-3, Methyl
2-ethylhexanoate 931-17-9, 1,2-Cyclohexanediol 1120-28-1, Methyl
eicosanoate 2226-96-2, 4-Hydroxy-2,2,6,6-tetramethylpiperidine
1-oxyl 2370-88-9, 1,3,5,7-Tetramethylcyclotetrasiloxane
2516-92-9, Bis(1-oxyl-2,2,6,6-tetramethylpiperidin-4-yl) sebacate
2896-70-0, 2,2,6,6-Tetramethyl-4-piperidinone 1-oxyl 3068-00-6,
1,2,4-Butanetriol 4704-94-3, Tris(hydroxymethyl)methane
10563-26-5, N,N'-Bis(3-aminopropyl)ethylenediamine
179552-48-8 **290821-91-9** 290822-02-5

(stabilizer precursor; hydroxy-substituted, N-alkoxy, hindered
heterocyclic amines for stabilizers for thermoplastic polymers
and coatings)

L42 ANSWER 5 OF 8 HCA COPYRIGHT 2007 ACS on STN

131:45141 Development of a Universal **Alkoxyamine** for "Living"
Free Radical Polymerizations. Benoit, Didier; Chaplinski, Vladimir;
Braslau, Rebecca; Hawker, Craig J. (NSF Center for Polymeric
Interfaces and Macromolecular Assemblies, IBM Almaden Research
Center, San Jose, CA, 95120-6099, USA). Journal of the American
Chemical Society, 121(16), 3904-3920 (English) 1999. CODEN: JACSAT.
ISSN: 0002-7863. Publisher: American Chemical Society.

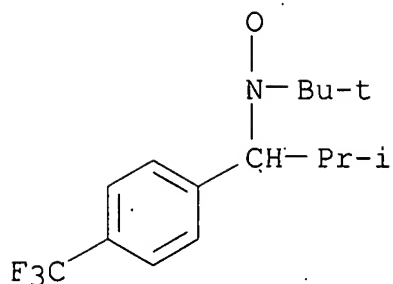
AB Examn. of novel **alkoxyamines** has demonstrated the pivotal
role that the nitroxide plays in mediating the "living" or
controlled polymn. of a wide range of vinyl monomers. Surveying a
variety of different **alkoxyamine** structures led to
 α -hydrido derivs. based on a 2,2,5-trimethyl-4-phenyl-3-
azahexane-3-oxy, 1, skeleton which were able to control the polymn.
of styrene, acrylate, acrylamide, and acrylonitrile based monomers.
For each monomer set, the mol. wt. could be controlled from 1000 to
200,000 amu with polydispersities typically 1.05-1.15. Block and
random copolymers based on combinations of the above monomers could
also be prepd. with similar control. In comparison with
2,2,6,6-tetramethylpiperidinoxyl (TEMPO), these new systems represent
a dramatic increase in the range of monomers that can be polymd.
under controlled conditions and overcome many of the limitations
assocd. with nitroxide-mediated "living" free radical procedures.
Monomer selection and functional group compatibility now approach
those of ATRP-based systems.

IT **226999-86-6P 226999-92-4P**

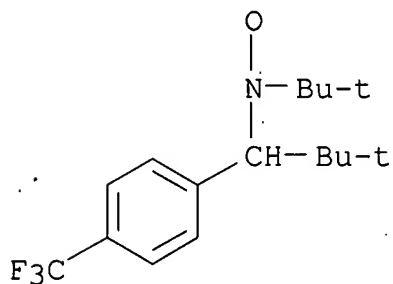
(in **alkoxyamine** prepn.; **alkoxyamine**-mediated
living free radical polymn. of styrene and acrylic compds.)

RN 226999-86-6 HCA

CN Nitroxide, 1,1-dimethylethyl 2-methyl-1-[4-
(trifluoromethyl)phenyl]propyl (9CI) (CA INDEX NAME)



RN 226999-92-4 HCA
 CN Nitroxide, 1,1-dimethylethyl 2,2-dimethyl-1-[4-(trifluoromethyl)phenyl]propyl (9CI) (CA INDEX NAME)



CC 35-3 (Chemistry of Synthetic High Polymers)
 ST **alkoxyamine** mediated living radical polymn styrene acrylate; catalyst **alkoxyamine** living radical polymn styrene acrylate
 IT Amines, preparation
 (alkoxy; **alkoxyamine**-mediated living free radical polymn. of styrene and acrylic compds.)
 IT Polymerization
 Polymerization catalysts
 (living, radical; **alkoxyamine**-mediated living free radical polymn. of styrene and acrylic compds.)
 IT 132416-36-5 154554-67-3 183194-54-9 188491-78-3 219908-58-4
 219908-68-6 224575-62-6 224967-65-1 227000-59-1 227000-69-3
 227000-79-5 227000-80-8 227000-81-9 227000-83-1 227000-84-2
 227000-85-3 227000-86-4 227000-87-5 227000-88-6 227000-89-7
 227000-90-0
 (**alkoxyamine**-mediated living free radical polymn. of styrene and acrylic compds.)
 IT 9003-49-0P, Poly(n-butyl acrylate) 9003-53-6P, Polystyrene
 9003-54-7P, Acrylonitrile-styrene copolymer 25014-41-9P,
 Acrylonitrile homopolymer 25034-86-0P, Methyl methacrylate-styrene
 copolymer 25119-83-9P, Acrylic acid-butyl acrylate copolymer
 25567-76-4P, Acrylonitrile-butyl acrylate copolymer 25767-47-9P,

n-Butyl acrylate-styrene copolymer 26222-39-9P,
 2-(N,N-Dimethylamino)ethyl methacrylate-styrene copolymer
 26793-34-0P, N,N-Dimethylacrylamide homopolymer 29760-26-7P,
 N,N-Dimethylacrylamide-styrene copolymer 32409-50-0P, Butyl
 acrylate-2-hydroxyethyl acrylate copolymer 33775-27-8P, Butyl
 acrylate-2-(2-methoxyethoxy)ethyl acrylate copolymer 50733-27-2P,
 Butyl acrylate-N,N-dimethylacrylamide copolymer 64171-34-2P, Butyl
 acrylate-glycidyl acrylate copolymer 106392-91-0P,
 2,2,3,3,4,4,4-Heptafluorobutyl acrylate-styrene copolymer
 110772-34-4P, Butyl acrylate-styrene block copolymer 226999-65-1P,
 Butyl acrylate-2,2,3,3,4,4,4-heptafluorobutyl acrylate copolymer
 (**alkoxyamine**-mediated living free radical polymn. of
 styrene and acrylic compds.)

IT 75-77-4, reactions 76-39-1 78-84-2, Isobutyraldehyde 79-46-9,
 2-Nitropropane 108-86-1, Phenyl bromide, reactions 344-04-7,
 Bromopentafluorobenzene 402-43-7, p-Trifluoromethylphenyl bromide
 554-12-1, Methyl propionate 585-71-7, 1-Bromoethylbenzene
 594-70-7, 2-Methyl-2-nitropropane 630-19-3, Pivalaldehyde
 762-04-9, Diethyl phosphite 937-14-4, m-Chloroperbenzoic acid
 1432-48-0 1592-20-7, p-Vinylbenzyl chloride 2154-70-3
 16302-61-7 174153-12-9 175093-20-6 182190-80-3

(in **alkoxyamine** prepn.; **alkoxyamine**-mediated
 living free radical polymn. of styrene and acrylic compds.)

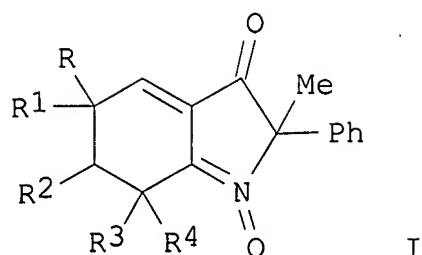
IT 53544-93-7P 56859-56-4P 61015-94-9P 72331-68-1P 85664-55-7P
 140116-61-6P 140116-62-7P 188526-94-5P **226999-86-6P**
226999-92-4P 226999-99-1P 227000-10-4P 227000-16-0P
 227000-22-8P 227000-39-7P 227000-46-6P

(in **alkoxyamine** prepn.; **alkoxyamine**-mediated
 living free radical polymn. of styrene and acrylic compds.)

L42 ANSWER 6 OF 8 HCA COPYRIGHT 2007 ACS on STN

129:54023 On the reaction of aminoxyls with dioxiranes. Dinoui, Anna;
 Curci, Ruggero; Carloni, Patricia; Damiani, Elisabetta; Stipa,
 Pierluigi; Greci, Lucedio (Dipartimento Chimica, Universita Bari,
 Bari, I-70126, Italy). European Journal of Organic Chemistry (5),
 871-876 (English) 1998. CODEN: EJOCFK. ISSN: 1434-193X.
 Publisher: Wiley-VCH Verlag GmbH.

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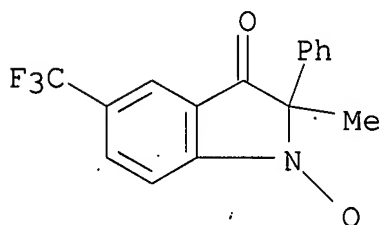
AB In the reactions of dimethyldioxirane and (trifluoromethyl)methyldioxirane with 2,2,6,6-tetramethylpiperidinyloxy (TEMPO) in Me₂CO, 1-methoxy-2,2,6,6-tetramethylpiperidine is produced in $\geq 98\%$ yield, both in air and under N₂, and in the absence or presence of a hydrocarbon (adamantane). Kinetic expts. show that TEMPO triggers the radical decompn. of the dioxirane, in addn. to scavenging Me radicals derived therefrom. The reactions of an aminoxyl less prone to oxidn., namely 1,2-dihydro-2-methyl-2-phenyl-3H-indol-3-one-1-oxy, with the above dioxiranes was also studied. In these cases, not only the corresponding **methoxyamine** is produced (12-16% yield), but quinonimine N-oxides I (RR₁ = O, R₂R₃ = bond, R₄ = H; R = H, R₁R₂ = bond, R₃R₄ = O; 12-21% and 18-19% yield, resp.) are also formed. Furthermore, significant amts. (8-14%) of the corresponding amine can be isolated. These observations provide useful information concerning the free-radical mechanism that follows the initial attack by the aminoxyl at the dioxirane.

IT **208452-81-7P**

(ESR as intermediate in reaction of aminoxyls with dioxiranes)

RN 208452-81-7 HCA

CN 1H-Indol-1-yloxy, 2,3-dihydro-2-methyl-3-oxo-2-phenyl-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



CC 22-4 (Physical Organic Chemistry)
Section cross-reference(s): 27

IT **208452-81-7P**

(ESR as intermediate in reaction of aminoxyls with dioxiranes)

L42 ANSWER 7 OF 8 HCA COPYRIGHT 2007 ACS on STN

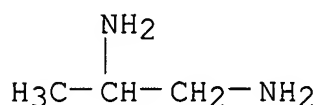
108:15150 Developments in the synthesis and reactivity of encapsulated metal ions. Sargeson, Alan M. (Res. Sch. Chem., Aust. Natl. Univ., Canberra, 2601, Australia). Pure and Applied Chemistry, 58(11), 1511-22 (English) 1986. CODEN: PACHAS. ISSN: 0033-4545.

AB The use of the template method is discussed to make larger and smaller cavity sizes of encapsulating ligands. The effect of cavity size and stereochem. on redox potentials and electron transfer reactions is discussed. Modification of the cages by oxidn. of the ligand to hydroxylamines, imines, amides and arom. systems is discussed. Mechanisms of demetalation from the cages are discussed.

IT 78-90-0, 1,2-Propanediamine
(capping reaction of cobalt-coordinated)

RN 78-90-0 HCA

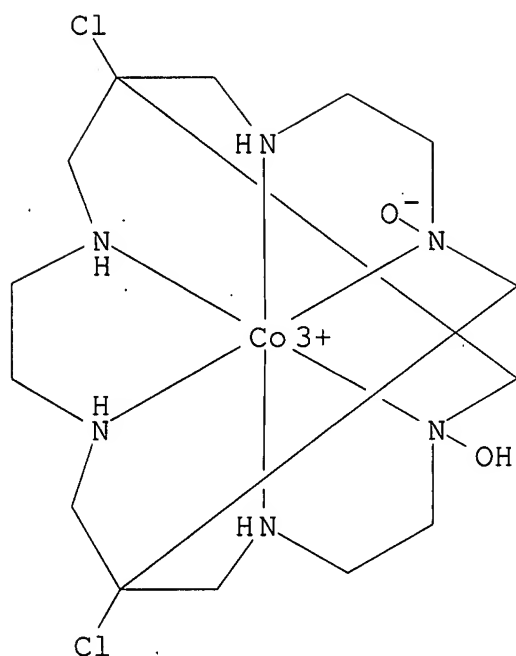
CN 1,2-Propanediamine (CA INDEX NAME)



IT 111231-63-1
(elec. potential of)

RN 111231-63-1 HCA

CN Cobalt(2+), (1,8-dichloro-3,10-dihydroxy-3,6,10,13,16,19-hexaazabicyclo[6.6.6]eicosanato-N3,N6,N10,N13,N16,N19)-, (OC-6-26)-(9CI) (CA INDEX NAME)



- CC 78-7 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 67
- IT Oxidation
 (of hexaazabicycloeicosane-type ligand in **transition metal** complexes)
- IT Demetalation
 Kinetics of demetalation
 (of **transition metal** hexaazabicycloeicosane complexes)
- IT **Transition metals**, compounds
 (hexaazabicycloeicosane complexes, prepn. and reactivity of)
- IT **78-90-0**, 1,2-Propanediamine
 (capping reaction of cobalt-coordinated)
- IT **111231-63-1**
 (elec. potential of)

L42 ANSWER 8 OF 8 HCA COPYRIGHT 2007 ACS on STN
 74:82635 Palladium(II) chelate complexes derived from
 3-hydroxyimino-2,4-pentane dione and some related complexes. White,
 Donald Andrew (Cent. Res. Dep., E.I. du Pont de Nemours and Co.,
 Wilmington, DE, USA). Journal of the Chemical Society [Section] A:
 Inorganic, Physical, Theoretical (2), 233-43 (English) 1971. CODEN:
 JCSIAP. ISSN: 0022-4944.

AB NO reacts with bis(2,4-pentanedionato)-palladium giving a mixt. of
 3-hydroxyimino-2,4-pentanedionato (2,4-pentanedionato)palladium and
 bis(3-hydroxyimino-2,4-pentanedionato)palladium. More convenient

routes to both these compds. are discussed. An analog of the latter compd. derived from Et 2-hydroxyimino-3-oxobutyrate is described. The chemistry and spectra of these complexes are discussed in relation to their structures.

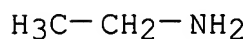
IT **75-04-7DP**, Ethylamine, palladium complexes

31317-75-6P

(prepn. of)

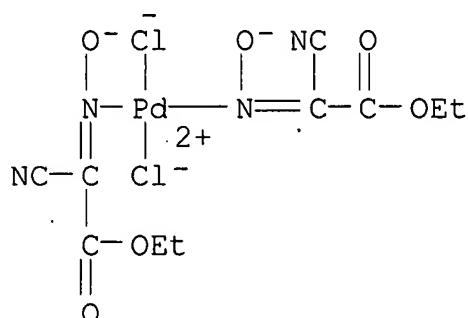
RN 75-04-7 HCA

CN Ethanamine (CA INDEX NAME)



RN 31317-75-6 HCA

CN Palladate(2-), dichlorobis(hydrogen cyanoglyoxylic acid 2-oximate)-, disodium, diethyl ester (8CI) (CA INDEX NAME)



● 2 Na⁺

CC 78 (Inorganic Chemicals and Reactions)

IT **75-04-7DP**, Ethylamine, palladium complexes 123-54-6DP,
2,4-Pentanedione, palladium complexes 603-32-7DP, Arsine,
triphenyl-, palladium complexes 603-35-0DP, Phosphine, triphenyl-,
palladium complexes 880-12-6DP, 2-Pentanone, 4-(phenylimino)-,
palladium complexes 1118-71-4DP, 3,5-Heptanedione,
2,2,6,6-tetramethyl-, palladium complexes 1663-45-2DP, Phosphine,
ethylenebis[diphenyl-, palladium complexes 3849-21-6DP, Glyoxylic
acid, cyano-, ethyl ester, 2-oxime, palladium complexes
5408-04-8DP, Butyric acid, 2,3-dioxo-, ethyl ester, 2-oxime,
platinum metal complexes 6028-98-4DP, Butyric acid, 2,3-dioxo-,
ethyl ester, 2-oxime 3-phenylhydrazone, palladium complexes
15214-40-1P 15636-06-3P 29917-12-2DP, 2,3,4-Pentanetrione,
3-oxime, **transition metal** complexes
31255-84-2P 31314-72-4P 31314-73-5P 31314-74-6P 31314-75-7P

31314-76-8P 31314-77-9P 31314-78-0P 31314-79-1P 31314-80-4P
 31314-81-5P 31314-82-6P 31314-83-7P 31314-84-8P 31317-73-4P
 31317-74-5P **31317-75-6P** 31317-76-7P 31317-77-8P
 31317-78-9P 31317-79-0P 31317-80-3P 31317-81-4P 31317-82-5P
 31317-84-7P 31396-81-3P 31396-82-4P 31396-83-5P 31398-00-2P
 31471-08-6P 32506-90-4P 98092-19-4DP, 2,3-Pentanedione,
 4-imino-, 3-oxime, palladium complexes 143996-86-5DP,
 2,3-Pentanedione, 4-(methylimino)-, 3-oxime, palladium complexes
 143996-87-6DP, 2,3-Pentanedione, 4-(ethylimino)-, 3-oxime, platinum
 metal complexes 145068-80-0DP, 2,3-Pentanedione, 4-(butylimino)-,
 3-oxime, palladium complexes
 (prepn. of)

=> D HIS L43-

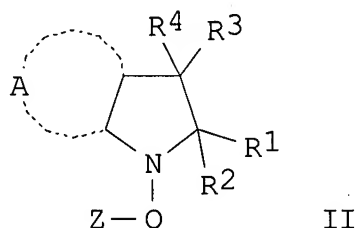
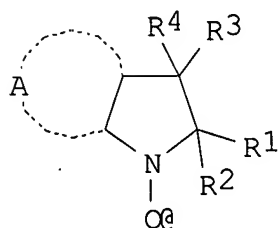
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L43 10126 S NITROXIDE#
 L44 6 S L43 AND (L24 OR L25) AND L14
 L45 24 S L43 AND (L24 OR L25) AND (L31 OR L38)
 L46 20 S L45 AND L24
 L47 6 S L44 NOT L42
 L48 20 S L45 NOT (L42 OR L47)
 L49 14 S 1840-2002/PY, PRY AND L48

=> D L47 1-6 CBIB ABS HITSTR HITIND

L47 ANSWER 1 OF 6 HCA COPYRIGHT 2007 ACS on STN
 147:10361 Controlled radical (co)polymerization of methacrylic acid or
 salts and/or methacrylate esters. Couturier, Jean Luc; Guillaneuf,
 Yohann; Bertin, Denis; Gigmes, Didier (Arkema, Fr.). Fr. Demande FR
 2893620 A1 20070525, 47pp. (French). CODEN: FRXXBL. APPLICATION:
 FR 2005-53590 20051124.

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AB Controlled radical (co)polymn. of the title compds. is effected in the presence of amino oxides I (A = hydrocarbon chain forming an arom. ring with the 2 atoms of the adjacent ring, optionally substituted by (substituted) cyclic or noncyclic groups, R1-4 = OH or org. group) or **alkoxyamines** II [A, R1-4 = same as in I, Z = CR8R9R10, R8, R9 = (substituted) alkyl, R10 = (substituted) alkenyl, (substituted) aryl, (substituted) aralkyl, CN, or CO2R11, R11 = H, Li, Na, K, NH4, (substituted) alkyl, (substituted) alkenyl, (substituted) aryl, or (substituted) aralkyl]. II are manufd. by treating I with ZX (Z = same as above, X = halo) in the presence of **transition metal** halides and amines.

CC 35-4 (Chemistry of Synthetic High Polymers)

IT **Nitroxides**

(controlled radical (co)polymn. of methacrylic acid or salts and/or methacrylate esters in presence of arom. pyrrolidine oxide derivs. or arom. pyrrolidinooxy derivs.)

IT **Transition metal** halides

(pyrrolidinooxy deriv. manufg. catalyst; controlled radical (co)polymn. of methacrylic acid or salts and/or methacrylate esters in presence of arom. pyrrolidine oxide derivs. or arom. pyrrolidinooxy derivs.)

L47 ANSWER 2 OF 6 HCA COPYRIGHT 2007 ACS on STN

147:9806 Process for preparation of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymerization (ATRP) initiator and a **nitroxide** or **nitroxide** precursor..

Matyjaszewski, Krzysztof; Spanswick, James (Carnegie Mellon University, USA). PCT Int. Appl. WO 2007059350 A2 20070524, 33pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IS, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2006-US44931 20061117. PRIORITY: US 2005-737545P 20051117.

AB A process for the prepn. of **alkoxyamines** comprises reaction of an ATRP initiator and a **nitroxide** in a reaction medium comprising a reducing agent and ≥ 1 **transition metal** catalyst. Thus, a mixt. of Et 2-bromoisobutyrate, TEMPO, CuBr2, dNbpy, and PhMe was deoxygenated, heated to 60°, and treated with a PhMe soln. of tin 2-ethylhexanoate to give after 14 h complete conversion to Et 2-(2,2,6,6-tetramethylpiperidyl)isobutyrate.

- IC ICM C07C
- CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
- ST **alkoxyamine** prepn; ATRP initiator **nitroxide**
transition metal catalyst reaction;
 bromoisobutyrate TEMPO coupling copper catalyst;
 piperidyloxyisobutyrate prepn
- IT Cyclization
 (prepn. of **alkoxyamines** via a coupling reaction using a
transition metal catalyst, an atom transfer
 radical polymn. (ATRP) initiator and a **nitroxide** or
nitroxide precursor)
- IT **Transition metals**, uses
 (prepn. of **alkoxyamines** via a coupling reaction using a
transition metal catalyst, an atom transfer
 radical polymn. (ATRP) initiator and a **nitroxide** or
nitroxide precursor)
- IT Hydroxylamines
 (prepn. of **alkoxyamines** via a coupling reaction using a
transition metal catalyst, an atom transfer
 radical polymn. (ATRP) initiator and a **nitroxide** or
nitroxide precursor)
- IT **Nitroxides**
 (prepn. of **alkoxyamines** via a coupling reaction using a
transition metal catalyst, an atom transfer
 radical polymn. (ATRP) initiator and a **nitroxide** or
nitroxide precursor)
- IT Reaction mechanism
 (radical; prepn. of **alkoxyamines** via a coupling
 reaction using a **transition metal** catalyst,
 an atom transfer radical polymn. (ATRP) initiator and a
nitroxide or **nitroxide** precursor)
- IT Aldehydes, reactions
 Monosaccharides
 Thiols, reactions
 (reducing agents; prepn. of **alkoxyamines** via a coupling
 reaction using a **transition metal** catalyst,
 an atom transfer radical polymn. (ATRP) initiator and a
nitroxide or **nitroxide** precursor)
- IT Carbohydrates, reactions
 (reducing sugars, reducing agents; prepn. of **alkoxyamines**
 via a coupling reaction using a **transition**
metal catalyst, an atom transfer radical polymn. (ATRP)
 initiator and a **nitroxide** or **nitroxide**
 precursor)
- IT 301-10-0
 (initiator; prepn. of **alkoxyamines** via a coupling
 reaction using a **transition metal** catalyst,
 an atom transfer radical polymn. (ATRP) initiator and a

- nitroxide or nitroxide precursor)**
- IT 7789-45-9, Cupric bromide 142646-58-0, 4,4'-Dinonyl-2,2'-bipyridine
(prepn. of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymn. (ATRP) initiator and a **nitroxide or nitroxide precursor**)
- IT 212128-91-1P
(prepn. of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymn. (ATRP) initiator and a **nitroxide or nitroxide precursor**)
- IT 600-00-0, Ethyl 2-bromoisobutyrate 2564-83-2, Tempo
(prepn. of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymn. (ATRP) initiator and a **nitroxide or nitroxide precursor**)
- IT 7681-38-1, Sodium hydrogen sulfate
(prepn. of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymn. (ATRP) initiator and a **nitroxide or nitroxide precursor**)
- IT 50-81-7, Ascorbic acid, reactions 50-99-7, Glucose, reactions 60-24-2, Mercaptoethanol 116-09-6, Hydroxyacetone 123-54-6, Acetylacetone, reactions 3144-16-9, Camphorsulfonic acid 15438-31-0, Fe²⁺, reactions 16043-45-1, Ti⁴⁺, reactions 16065-83-1, Cr³⁺, reactions 22537-23-1, Al³⁺, reactions 22541-75-9, Ti³⁺, reactions 22541-90-8, Sn²⁺, reactions
(reducing agent; prepn. of **alkoxyamines** via a coupling reaction using a **transition metal** catalyst, an atom transfer radical polymn. (ATRP) initiator and a **nitroxide or nitroxide precursor**)

L47 ANSWER 3 OF 6 HCA COPYRIGHT 2007 ACS on STN

139:86082 **Transition metal**-catalyzed process for conversion of alkenes to sterically hindered substituted N-**alkoxyamines**. Pastor, Stephen Daniel; Shum, Sai Ping (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2003053931 A1 20030703, 50 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-EP14134 20021212. PRIORITY: US 2001-342330P 20011221; US 2002-409374P

20020909.

- AB Sterically hindered N-substituted alkyloxyamines useful as light stabilizers for polymers are prepd. from alkenes by **transition metal**-catalyzed reaction of an intermediate alkylborane with a sterically hindered nitroxyl radical. Thus, reacting a mixt. contg. 4-hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl 12.5, NaOH 37.5, AgNO₃ 18.8, and BEt₃ 4.2 mmol in water gave 87.6% 1-ethoxy-4-hydroxy-2,2,6,6-tetramethylpiperidine.
- IC ICM C07D211-94
ICS C07D207-46
- CC 37-2 (Plastics Manufacture and Processing)
Section cross-reference(s): 27
- IT Amines, preparation
(hindered; **transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT Light stabilizers
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT **Transition metal** compounds
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT **Nitroxides**
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT Alkenes, reactions
(α -, C18-30, C16-18; **transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT 6046-93-1, Copper(II) acetate monohydrate 7758-98-7, Copper sulfate, uses 7761-88-8, Silver nitrate, uses
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT 87018-00-6P 122586-66-7P 131807-04-0P, 1-Octyloxy-4-hydroxy-2,2,6,6-tetramethylpiperidine 156908-91-7P 554409-12-0P 554409-13-1P
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)
- IT 97-94-9, Triethylborane 110-83-8, Cyclohexene, reactions 122-56-5, Tributylborane 1088-01-3, Tricyclohexylborane 2226-96-2, 4-Hydroxy-2,2,6,6-tetramethylpiperidine-1-oxyl 2896-70-0, 4-Oxo-2,2,6,6-tetramethylpiperidine-1-oxyl 3248-78-0,

Trioctylborane 14691-89-5, 4-Acetoamido-2,2,6,6-tetramethylpiperidine-1-oxyl 21485-44-9, 2,5-Diethyl-2,5-dimethylimidazolidin-4-one-1-oxyl
(**transition metal**-catalyzed conversion of alkenes to sterically hindered substituted N-**alkoxyamines**)

L47 ANSWER 4 OF 6 HCA COPYRIGHT 2007 ACS on STN

137:295596 **Transition-metal**-catalyzed preparation of sterically hindered N-substituted **alkoxyamines** and compositions. Pastor, Stephen Daniel; Shum, Sai Ping (Ciba Specialty Chemicals Holding Inc., Switz.). PCT Int. Appl. WO 2002079182 A2 20021010, 43 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-EP3311 20020325. PRIORITY: US 2001-824145 20010402.

AB Sterically hindered N-substituted **alkoxyamine** stabilizers are prep'd. by the **transition-metal**-catalyzed decompn. of diazonium salts in the presence of a sterically hindered nitroxyl radical. These compds. are useful as thermal and light stabilizers for a variety of org. substrates. Pyridine is added to the reaction mixt. to increase reaction yield and solvency. Thus, a soln. of 1.95 g 1-oxyl-2,2,6,6-tetramethylpiperidine, 3.1 g tert-Bu nitrite and 7.5 mg (S,S)-(+)-N,N-bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanedi-aminocobalt(II) in 100 mL pyridine at 65-70° under N is added dropwise over 20 min. to a soln. of 5.6 g 2-allyloxylaniline in 20 mL pyridine, stirred 40 min. at 65-70°, and concd. to give 63.7% 1-(2,3-Dihydrobenzofuran-3-yl-methoxy)-2,2,6,6-tetramethylpiperidine stabilizer. Polypropylene is stabilized with the above compd.

IC ICM C07D307-80

ICS C07D405-12

CC 37-2 (Plastics Manufacture and Processing).
Section cross-reference(s): 27, 45

ST light stabilizer **alkoxyamine** prepn; heat stabilizer **alkoxyamine** prepn

IT Amines, preparation
(hindered, N-substituted, alkoxy; **transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)

IT Addition reaction catalysts

- (**transition metal** compds.; **transition metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT Candles
Heat stabilizers
Light stabilizers
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT **Transition metal** compounds
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT Waxes
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT Discoloration prevention agents
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine** for)
- IT 188264-84-8, (S,S)-(+) -N,N'-Bis(3,5-di-tert-butylsalicylidene)-1,2-cyclohexanediaminocobalt(II)
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT 79240-46-3P 468084-47-1P 468084-49-3P 468084-54-0P
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT 79240-47-4P
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT 110-86-1, Pyridine, uses
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT 9003-07-0, Polypropylene
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)
- IT 540-80-7D, allylaniline diazonium derivs. 2226-96-2,
1-Oxyl-2,2,6,6-tetramethyl-4-hydroxypiperidine 2406-25-9,
Di-tert-butyl **nitroxide** 2564-83-2, 1-Oxyl-2,2,6,6-tetramethylpiperidine 27096-64-6D, 2-Allyloxylaniline, diazonium butylnitrite derivs. 468084-46-0D, diazonium butylnitrite derivs. 468084-52-8D, diazonium butylnitrite derivs.
(**transition-metal**-catalyzed prepn. of sterically hindered N-substituted **alkoxyamine**)

L47 ANSWER 5 OF 6 HCA COPYRIGHT 2007 ACS on STN
136:169419 Method for preparing **alkoxyamines** from **nitroxides**. Couturier, Jean-Luc; Guerret, Olivier (ATOFINA, Fr.). PCT Int. Appl. WO 2002012149 A2 20020214, 24 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,

IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (French). CODEN: PIXXD2. APPLICATION: WO 2001-FR2526 20010802. PRIORITY: FR 2000-10344 20000804.

- AB The invention concerns a method for prepg. **alkoxyamines** in a biphasic medium. Said method consists in mixing an ionic liq. (such as 3-methyl-1-propylimidazolium bromide), an org. solvent, a **metal salt**, a ligand that complexes with the metal of the **metal salt**, a halohydrocarbon, and a **nitroxide**, maintaining the reaction medium under agitation at a temp. between 20°C and 90°C, until the **nitroxide** is eliminated, decanting, recuperating the org. phase; optionally washing it with water and then in isolating the **alkoxyamine** by evapg. the org. solvent under reduced pressure. This process allows improved recycling of the metal and ligand.
- IC ICM C07C
- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23
- ST **alkoxyamine** manuf **nitroxide** alkylation biphasic media; metal complex catalyst **nitroxide** alkylation media; halohydrocarbon **nitroxide** reaction biphasic media; methylpropylimidazolium bromide biphasic media **nitroxide** alkylation; ionic liq org solvent biphasic media **nitroxide** alkylation
- IT Solvents
(org.; prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT Alkylation
Alkylation catalysts
Ionic liquids
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT Metals, uses
Salts, uses
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT Alkyl halides
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT **Nitroxides**

- (prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 106-94-5, Propyl bromide 109-69-3, Butyl chloride 616-47-7, 1-Methylimidazole
(ionic liq. precursor; prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 79917-90-1P, 1-Butyl-3-methylimidazolium chloride 85100-76-1P, 3-Methyl-1-propylimidazolium bromide
(ionic liq.; prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 79917-89-8
(ionic liq.; prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 56-18-8 3030-47-5, PMDETA
(ligand; prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 7439-89-6D, Iron, halides 7440-02-0D, Nickel, halides 7440-50-8, Copper, uses 7440-50-8D, Copper, halides 7787-70-4, Cuprous bromide
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 224575-62-6P
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 108-88-3, Toluene, uses
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)
- IT 585-71-7, 1-Bromoethylbenzene 188526-94-5, N-tert-Butyl-1-diethylphosphono-2,2-dimethylpropyl **nitroxide**
(prepg. **alkoxyamines** from **nitroxides** by alkylation in ionic liq.-org. solvent biphasic system in presence of metals and ligands)

L47 ANSWER 6 OF 6 HCA COPYRIGHT 2007 ACS on STN

133:309685 Method for preparing **alkoxyamines** from **nitroxides**. Couturier, Jean-Luc; Guerret, Olivier; Senninger, Thierry (Elf Atochem S. A., Fr.). PCT Int. Appl. WO 2000061544 A1 20001019, 25 pp. DESIGNATED STATES: W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,

KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG.

(French). CODEN: PIXXD2. APPLICATION: WO 2000-FR750 20000324. PRIORITY: FR 1999-4405 19990408.

AB The invention concerns a method for prepg. **alkoxyamines** which consists in mixing in an org. solvent, a **metallic salt**, a **metal** ligand, a halo-carbon ZX compd., and a **nitroxide**; in maintaining the reaction medium stirred at a temp. ranging between 20 >C and 90 >C, until the **nitroxide** disappears; in recuperating the org. by evapg. the org. solvent under reduced pressure. E.g., reaction of TEMPO with PhCHBrMe in presence of Cu, CuBr and N,N,N',N',N''-pentamethyldiethylenetriamine gave 97% 1-(2,2,6,6-tetramethylpiperidinyloxy)-1-phenylethane.

IC ICM C07C239-20

CC 23-5 (Aliphatic Compounds)

ST **alkoxyamine** prepn **nitroxide**; amine alkoxy prepn **nitroxide**

IT Amines, preparation
(alkoxylated; prepn. of **alkoxyamines** from **nitroxides**)

IT **Nitroxides**
(prepn. of **alkoxyamines** from **nitroxides**)

IT 110-18-9 3030-47-5 3083-10-1 7787-70-4, Cuprous bromide
33527-91-2 41203-22-9 96556-05-7 133256-59-4
(prepn. of **alkoxyamines** from **nitroxides**)

IT 154554-67-3P 288583-75-5P 288583-77-7P 300811-93-2P
(prepn. of **alkoxyamines** from **nitroxides**)

IT 585-71-7, (1-Bromoethyl)benzene 2564-83-2, TEMPO 5445-17-0,
Methyl 2-bromopropionate 188526-94-5
(prepn. of **alkoxyamines** from **nitroxides**)

=> D L49 1-14 TI

L49 ANSWER 1 OF 14 HCA COPYRIGHT 2007 ACS on STN

TI Method of making crystalline nanoparticles from organometallic and **transition metal** complexes

L49 ANSWER 2 OF 14 HCA COPYRIGHT 2007 ACS on STN

TI **Nitroxides** inhibit peroxy radical-mediated DNA scission and enzyme inactivation

L49 ANSWER 3 OF 14 HCA COPYRIGHT 2007 ACS on STN

TI Metal complexes with nitronyl **nitroxide** substituted

phenolate ligands providing new magnetic exchange interaction pathways - synthesis, structures, magnetic dilution studies, and ab initio calculations

- L49 ANSWER 4 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Preparation of organic compounds having **nitroxide** free radicals
- L49 ANSWER 5 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI New chelating **nitroxide** free radical ligands for heterospin-magnetic engineering
- L49 ANSWER 6 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Cleaning of water filters with calcium-binding agents and catalytic oxidation in the presence of a di-tert-nitroxyl compound
- L49 ANSWER 7 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Inhibition of pulp and paper yellowing using **nitroxides** and other co-additives
- L49 ANSWER 8 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Coordination complexes in conducting and magnetic molecular materials
- L49 ANSWER 9 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Features of the diffusion of molecules and ions in solutions of complex forming polymers
- L49 ANSWER 10 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Nitrosylated and nitrated superoxide oxidants and reductants for preventing superoxide-mediated cell damage and for treating inflammatory disorders
- L49 ANSWER 11 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Gas-filled microspheres as magnetic resonance imaging (MRI) contrast agents
- L49 ANSWER 12 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI **Nitroxide** stable radicals protect beating cardiomyocytes against oxidative damage
- L49 ANSWER 13 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Paramagnetic probe for molecular interactions. Part III. EPR and sodium-23 NMR studies of ionic association and of sodium cation solvation by a **nitroxide** radical
- L49 ANSWER 14 OF 14 HCA COPYRIGHT 2007 ACS on STN
 TI Investigation of various solute-solute interactions from proton NMR

relaxation induced by paramagnetic solutes

=> D L49 4,9 CBIB ABS HITSTR HITIND

L49 ANSWER 4 OF 14 HCA COPYRIGHT 2007 ACS on STN

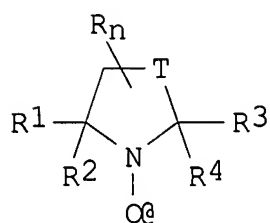
133:43449 Preparation of organic compounds having **nitroxide** free radicals. Iwazaki, Katsuhiko (Koei Chemical Co., Ltd., Japan).

PCT Int. Appl. WO 2000039093 A1 **20000706**, 15 pp.

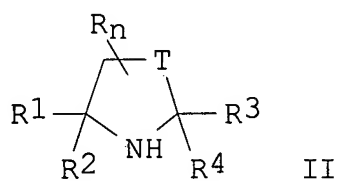
DESIGNATED STATES: W: US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (Japanese). CODEN: PIXXD2.

APPLICATION: WO 1999-JP7379 19991228. PRIORITY: JP 1998-374691 19981228.

GI



I



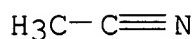
II

AB Title compds. I (T = methylene, ethylene, oxygen, or methyleneoxy; R = alkyl, aralkyl, aryl, cycloalkyl, alkoxy, acyl, acyloxy, amino, hydroxy, heterocycle; R1, R2, R3, R4 = alkyl, aryl; R1R2 and/or R3R4 = tetramethylene, pentamethylene; n = an integer of 0 to 6) are prepd. by reaction of sterically hindered, cyclic secondary amines II with peroxides in the presence of catalysts and cyano-contg. compds. Thus, reaction of 2,2,6,6-tetramethylpiperidine with H2O2 in MeCN in the presence of ammonium paratungstate gave 93.5% 2,2,6,6-tetramethylpiperidin-1-oxyl.

IT **75-05-8**, Acetonitrile, reactions **768-66-1**, 2,2,6,6-Tetramethylpiperidine (prepn. of org. compd. having **nitroxide** free radical)

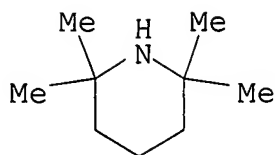
RN 75-05-8 HCA

CN Acetonitrile (CA INDEX NAME)



RN 768-66-1 HCA

CN Piperidine, 2,2,6,6-tetramethyl- (CA INDEX NAME)



- IC ICM C07D211-94
ICS C07B061-00
- CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
- ST **nitroxide** radical prepn; methylpiperidinoxyl prepn
- IT Organic compounds, reactions
(cyano; prepn. of org. compd. having **nitroxide** free radical by oxidn. of secondary amines in presence of cyano compds.)
- IT **Transition metals**, uses
(prepn. of org. compd. having **nitroxide** free radical by oxidn. of secondary amines in presence of cyano compds.)
- IT **Nitroxides**
(prepn. of org. compd. having **nitroxide** free radical by oxidn. of secondary amines in presence of cyano compds.)
- IT Peroxides, reactions
(prepn. of org. compd. having **nitroxide** free radical by oxidn. of secondary amines in presence of cyano compds.)
- IT Amines, reactions
(secondary, cyclic; prepn. of org. compd. having **nitroxide** free radical by oxidn. of secondary amines in presence of cyano compds.)
- IT 12028-06-7, Ammonium paratungstate
(prepn. of org. compd. having **nitroxide** free radical)
- IT 2564-83-2P, 2,2,6,6-Tetramethylpiperidin-1-oxyl
(prepn. of org. compd. having **nitroxide** free radical)
- IT **75-05-8**, Acetonitrile, reactions **768-66-1**, 2,2,6,6-Tetramethylpiperidine 7722-84-1, Hydrogen peroxide, reactions
(prepn. of org. compd. having **nitroxide** free radical)
- L49 ANSWER 9 OF 14 HCA COPYRIGHT 2007 ACS on STN
- 128:180893 Features of the diffusion of molecules and ions in solutions of complex forming polymers. Kokorin, A. I.; Pridantsev, A. A. (Inst. Khim. Fiz. im. Semenova, RAN, Moscow, Russia). Zhurnal Fizicheskoi Khimii, 71(12), 2171-2177 (Russian) **1997**. CODEN: ZFKHA9. ISSN: 0044-4537. Publisher: MAIK Nauka.
- AB ESR spectroscopy was used to study nitroxyl radical exchange with paramagnetic **transition metal** ions, Cu(II), Ni(II), Co(II), Mn(II), Zn(II), Cr(III), Fe(III). Based on the exchange date, diffusion in complex-forming polymers was studied. Spin rate exchange const. was detd. for polyethyleneamine and

partially alkylated poly(4-vinylpyridine) solns. in relation to ion elec. charge and charge and size of spin probe mol.

IT **9002-98-6**, Aziridine homopolymer
 (mol. and ion diffusion in solns. of complex forming polymers)
 RN 9002-98-6 HCA
 CN Aziridine, homopolymer (CA INDEX NAME)

CM 1

CRN 151-56-4

CMF C2 H5 N



CC 36-7 (Physical Properties of Synthetic High Polymers)

Section cross-reference(s): 35

ST polyethyleneamine soln diffusion **nitroxide** metal ion;
 alkylated polyvinylpyridine diffusion metal complexation; copper ion
 exchange **nitroxide** polymer soln; zinc ion exchange
nitroxide polymer soln; chromium ion exchange
nitroxide polymer soln; nickel ion exchange
nitroxide polymer soln; manganese ion exchange
nitroxide polymer soln; cobalt ion exchange
nitroxide polymer soln; iron ion exchange **nitroxide**
 polymer soln; nitroxyl radical metal ion exchange complexation

IT **Transition metals**, properties
 (ions; mol. and ion diffusion in solns. of complex forming
 polymers)

IT **Nitroxides**
 (mol. and ion diffusion in solns. of complex forming polymers)

IT Spin labels
 (**nitroxides**; mol. and ion diffusion in solns. of
 complex forming polymers)

IT 2154-68-9, 2,2,5,5-Tetramethyl-3-carboxypyrrolidine-N-oxyl
 2226-96-2, TEMPO OH 2564-83-2, TEMPO 4399-80-8 7439-89-6,
 Iron, properties 7439-96-5, Manganese, properties 7440-02-0,
 Nickel, properties 7440-47-3, Chromium, properties 7440-48-4,
 Cobalt, properties 7440-50-8, Copper, properties 7440-66-6,
 Zinc, properties **9002-98-6**, Aziridine homopolymer
 14691-88-4, 4-Amino-2,2,6,6-tetramethylpiperidine-N-oxyl
 25232-41-1D, Poly(4-vinylpyridine), partially Me or Et
 bromide-quaternized 31146-15-3, 4-(2'-Hydroxyethyl)-2,2,6,6-
 tetramethylpiperidine-N-oxyl 39753-74-7 54913-15-4
 (mol. and ion diffusion in solns. of complex forming polymers)